

Regional Chemical Modeling in Support of ICARTT

Topics:

- How good were the regional forecasts?
- What are we learning about the emissions?
- What are our plans for integrating models with observations?

Our Analysis Framework

MOZART Global Chemical Transport Model

Mesoscale Meteorological Model (RAMS or MM5)

**Influence Functions
Emission Biases/
Inversion**

**Meteorological
Dependent Emissions
(biogenic, dust, sea salt)**

**Anthropogenic &
biomass burning
Emissions**

TOMS O₃

**STEM Tracer Model
(classified tracers for
regional and emission types)**

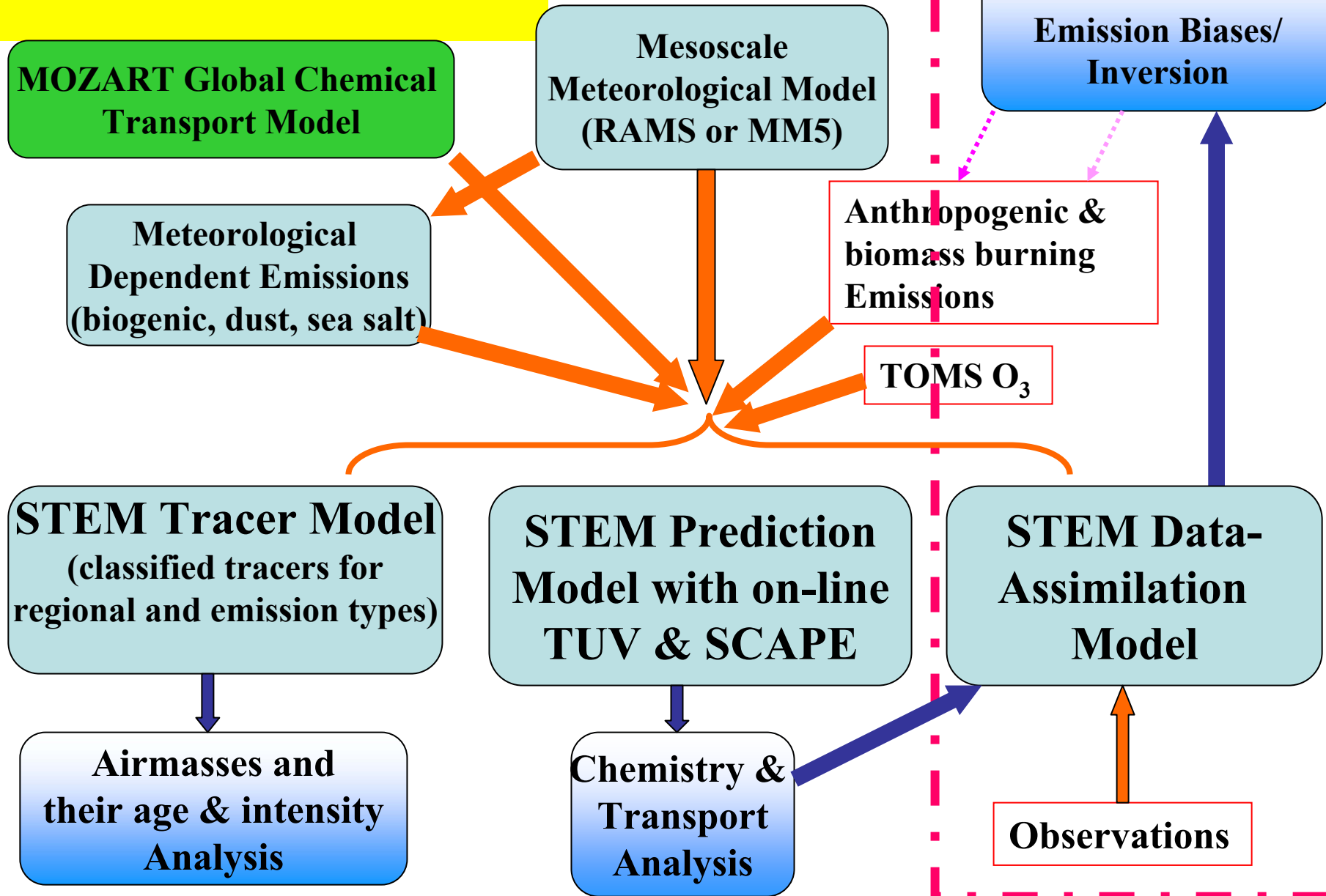
**STEM Prediction
Model with on-line
TUV & SCAPE**

**STEM Data-
Assimilation
Model**

**Airmasses and
their age & intensity
Analysis**

**Chemistry &
Transport
Analysis**

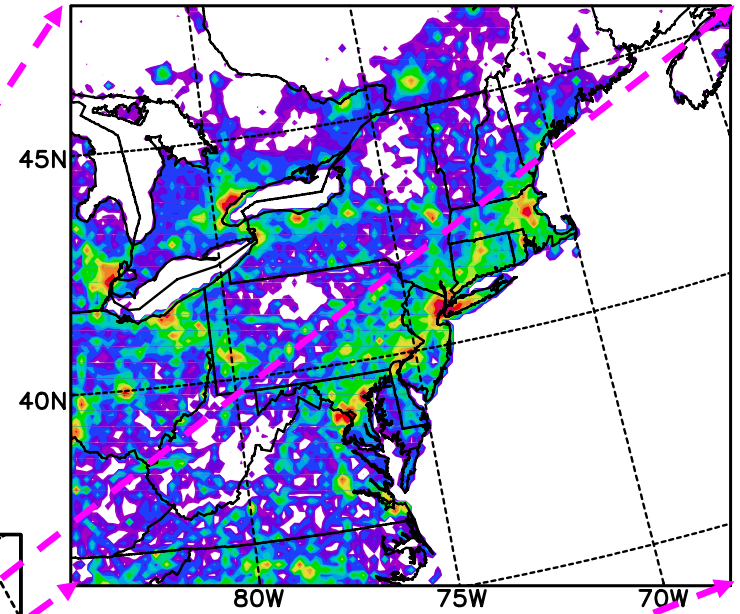
Observations



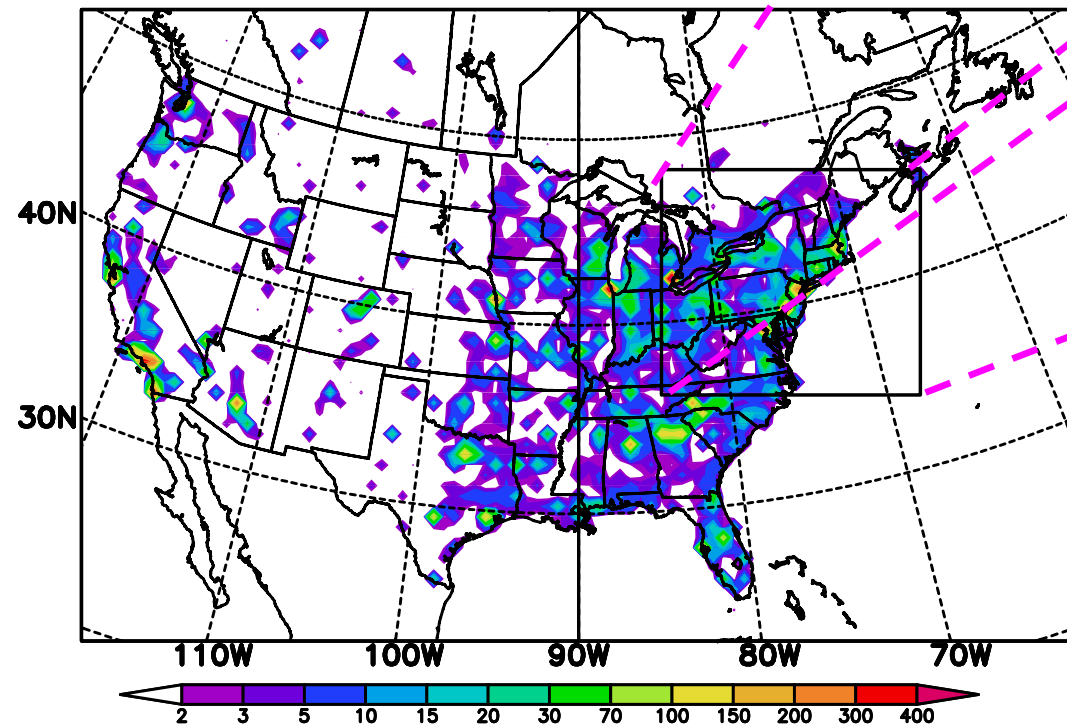
Analysis Done at 60 and 12 km Horizontal Resolution

NEI-1999 emission in 60km (below)
and 12km (right) domains.

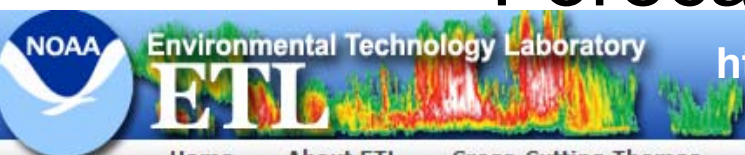
Mean CO Emission for Typical Summer day (10^{11} Molecules/cm²/s)



Mean CO Emission for Typical Summer day (10^{11} Molecules/cm²/s)



Extensive Real-Time Evaluation of Regional Forecasts – *Stu McKeen*



<http://www.etl.noaa.gov/programs/2004/neaqs/verification/>

Home About ETL Cross-Cutting Themes Programs & Projects Observing Systems Divisions

Program Links

NEAQS Home
Contact Us

Model Cycle

Select the model cycle
initialization:

00Z Jul 13
12Z Jul 13

Sites

Select site type:

- ☐ Profiler
☐ Chemistry
☒ Mobile

Select site location:

Ron Brown

Data Archive

Select a date:

July 2004

Sun	Mon	Tue	Wed	Thu	Fri	Sat
				1	2	3
4	5	6	7	8	9	10
11	12	13	14	15	16	17
18	19	20	21	22	23	24
25	26	27	28	29	30	31

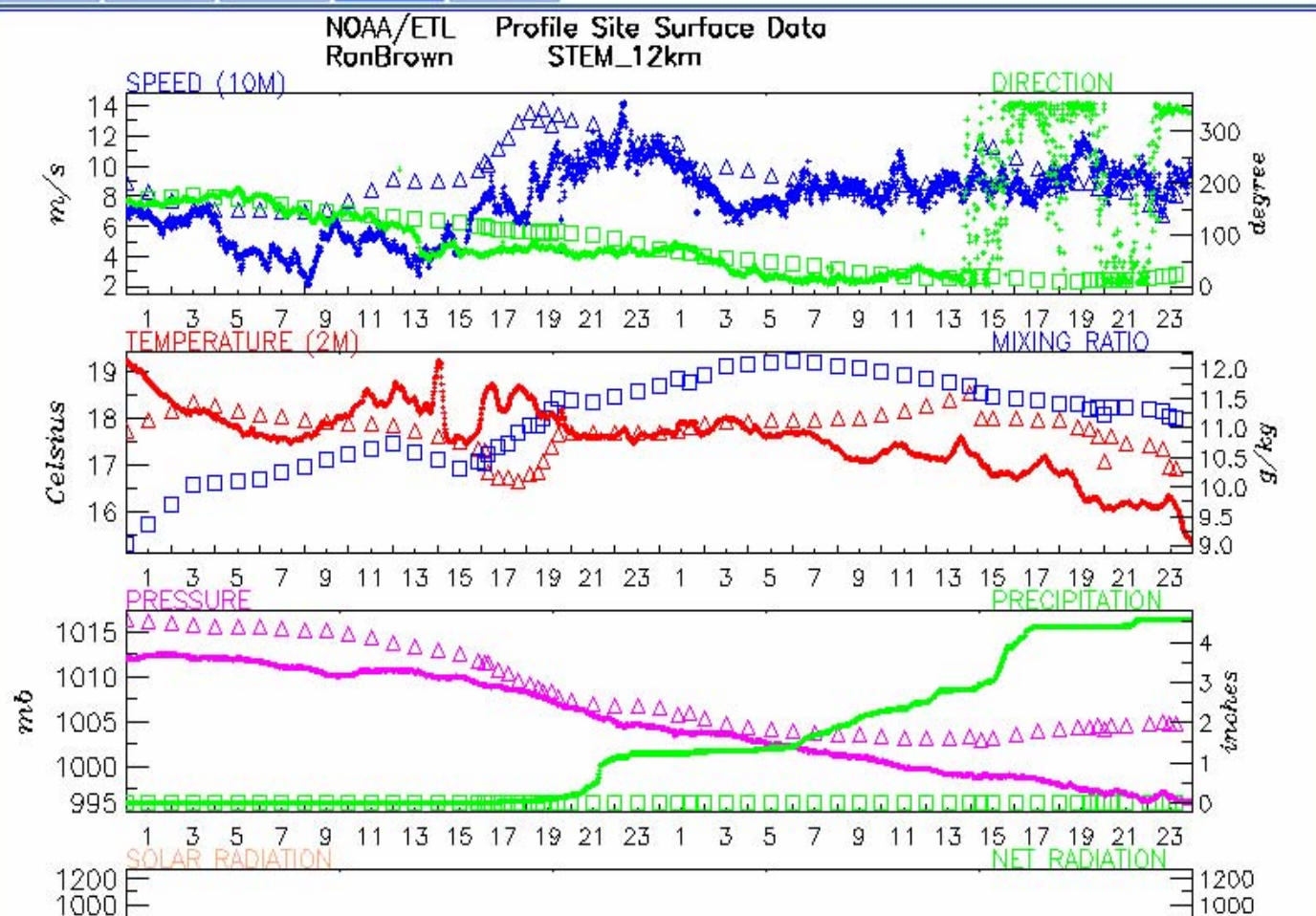
Page Updated:

Mon, 11 Oct 2004 16:24:32

GMT

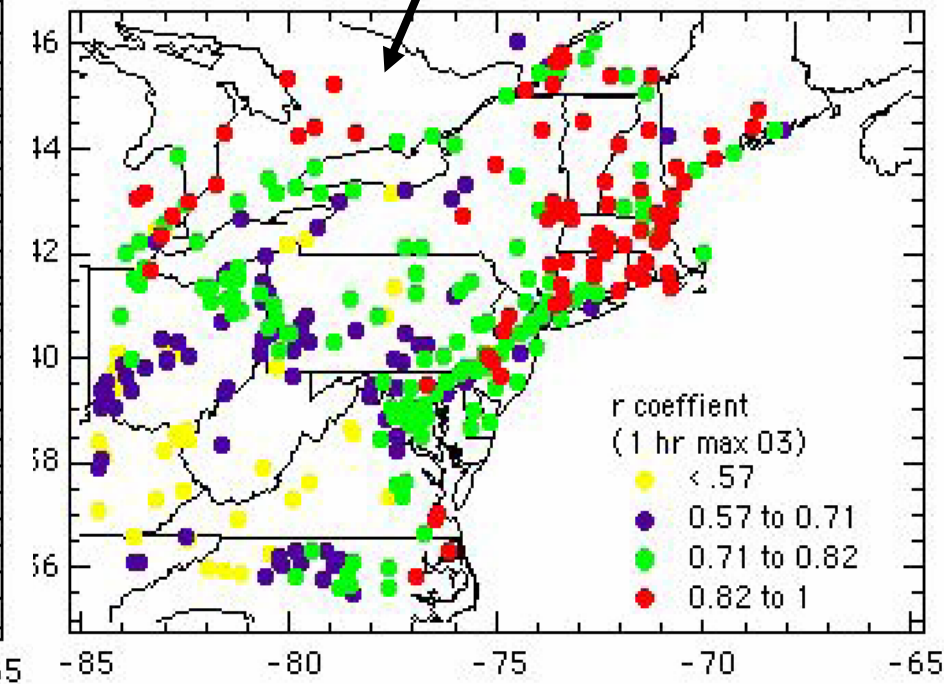
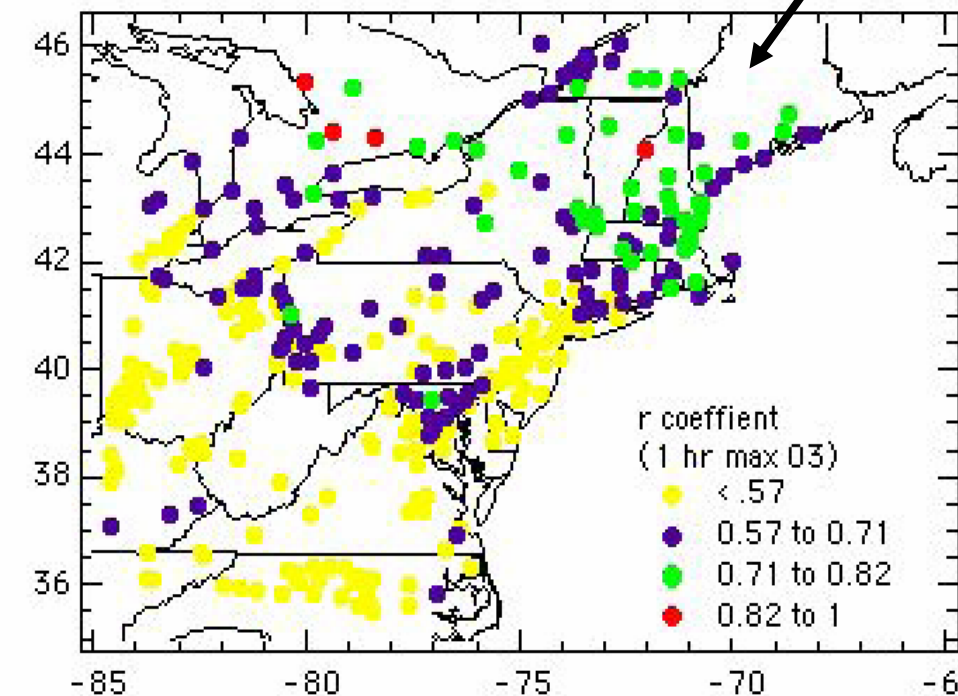
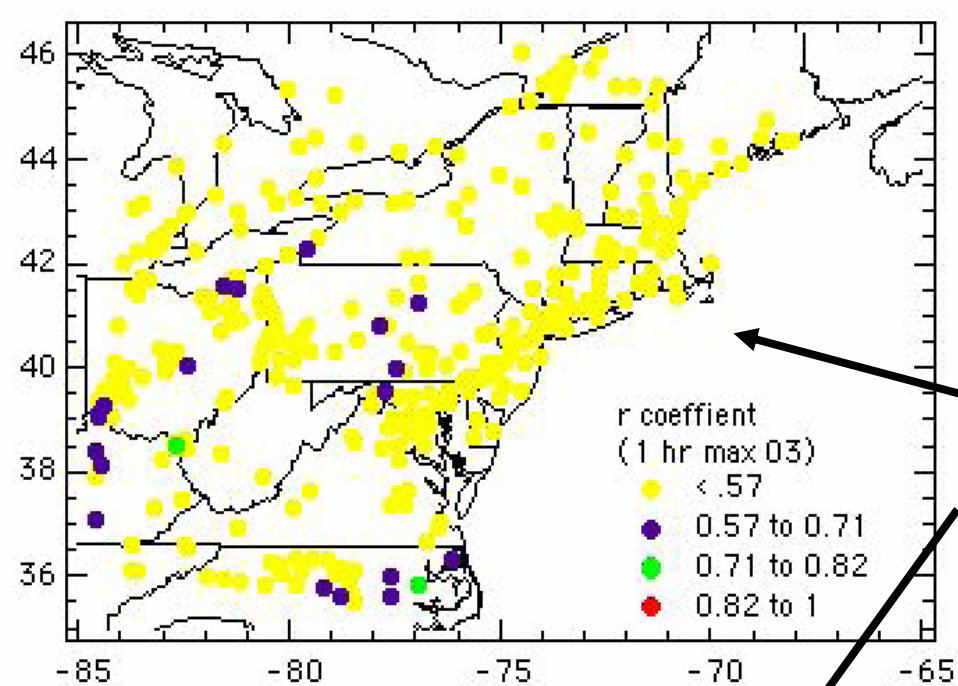
AURAMS-42 CHRONOS-21 Eta/CMAQ-12 WRF_1-27 WRF_2-27 WRF_2-12 BAMS-45 BAMS-15 STEM-12

SNR/Winds RASS/Winds O3 Profile Sfc Met Sfc Chem

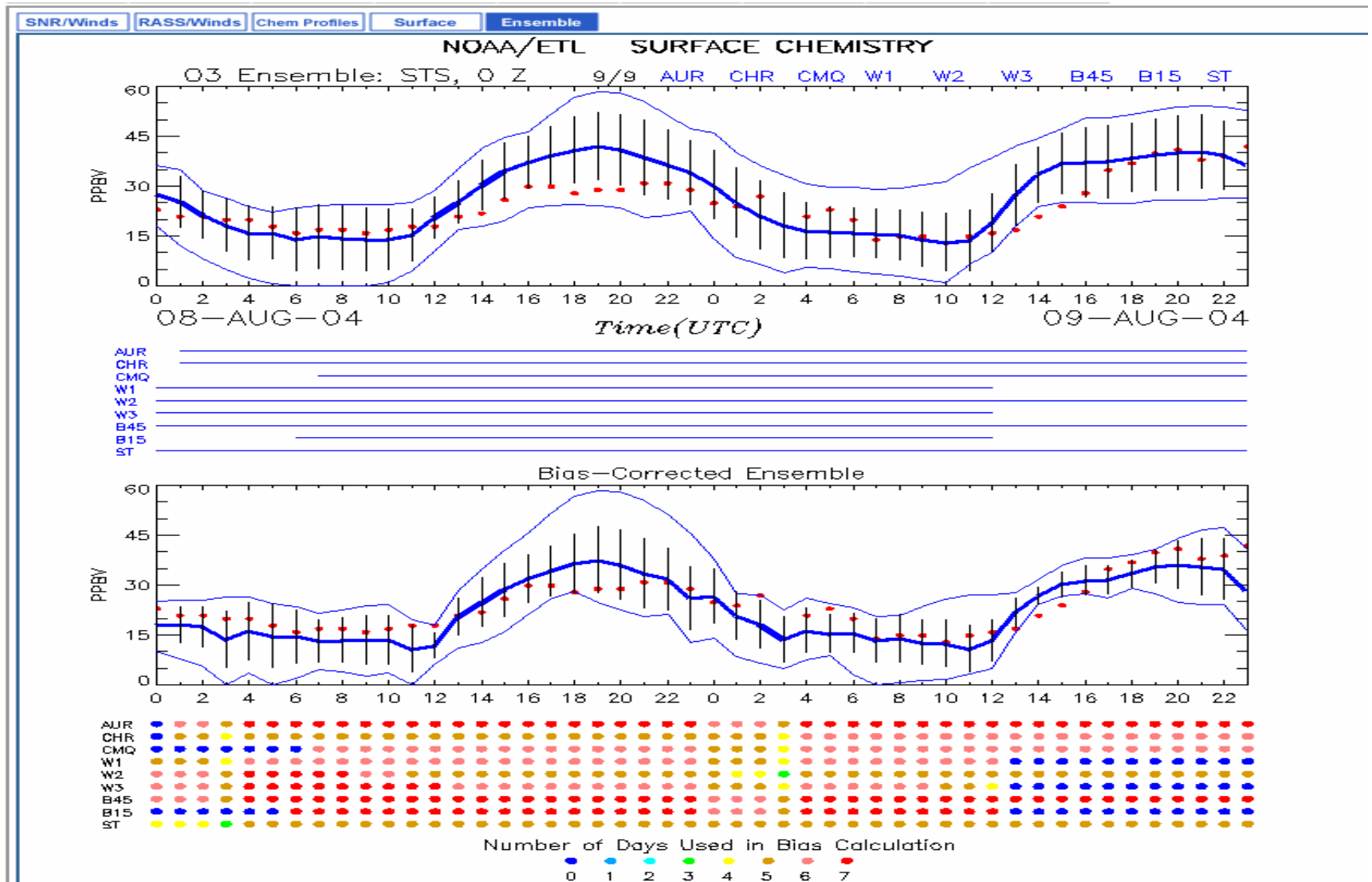


Complimentary Actions to Improve Our Ability to Forecast Pollution are Needed

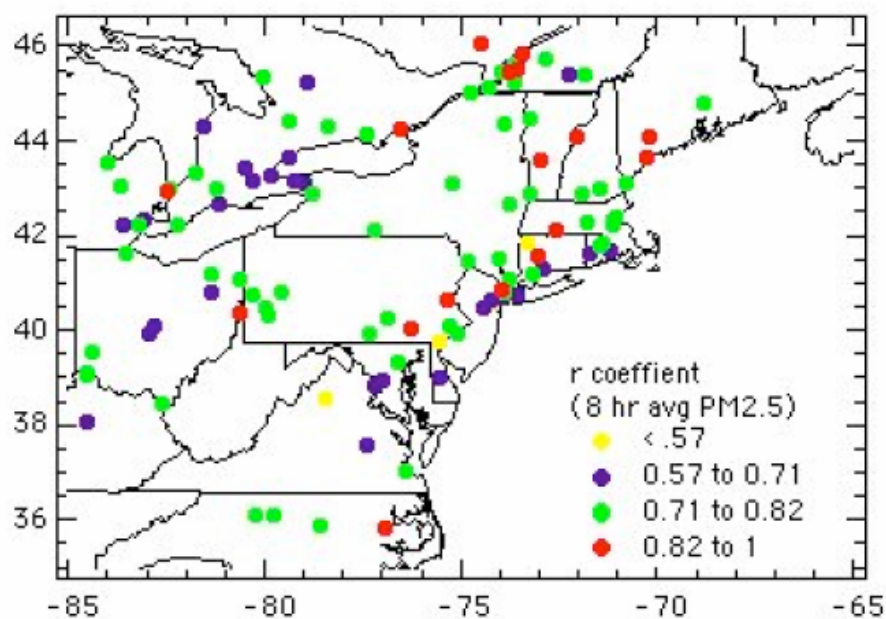
- * Persistence
- * Single Forward Model w/o assimilation
- * Ensemble forecast (8 models) w/o assimilation



Ensemble Techniques Help !



Ensemble Methods Also Work for PM2.5 Forecasting



Comparison Statistics for
Geometric Ensemble with
AIRNOW daily 8-hr avg PM2.5
7/14/04 through 8/18/04

	median average	
r coeff.	0.75	0.73
Md/Ob ratio	0.86	1.00
ratio RMSE	1.76	1.90
Sdev	5.55	5.84
Skill factor (%)	75.42	

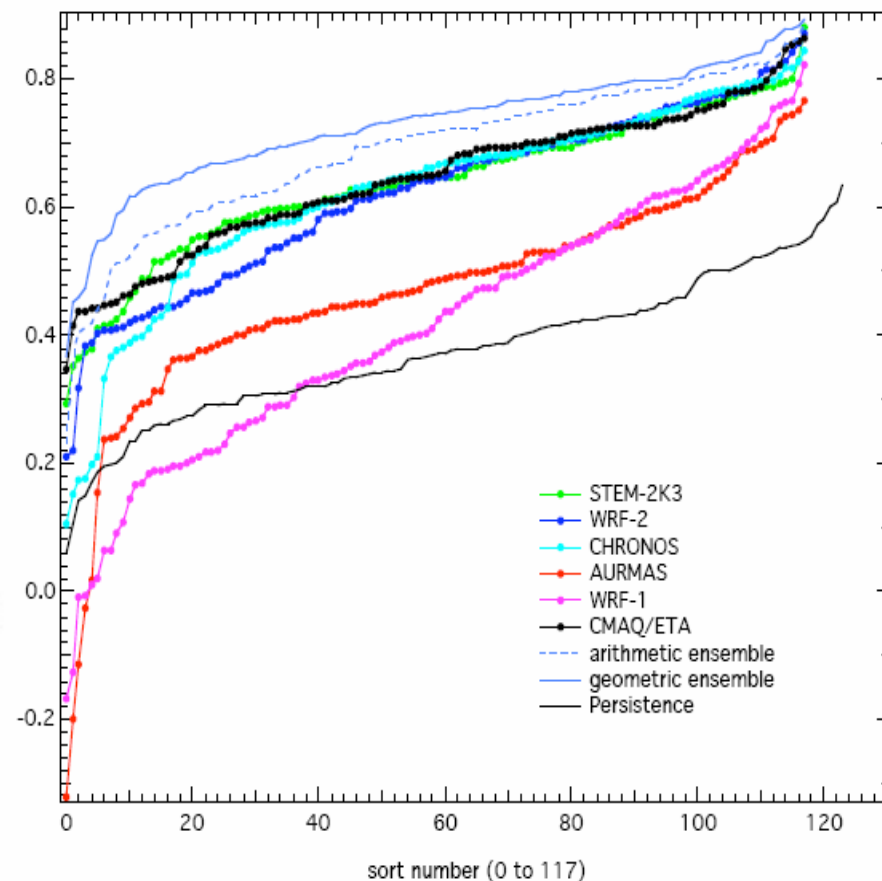
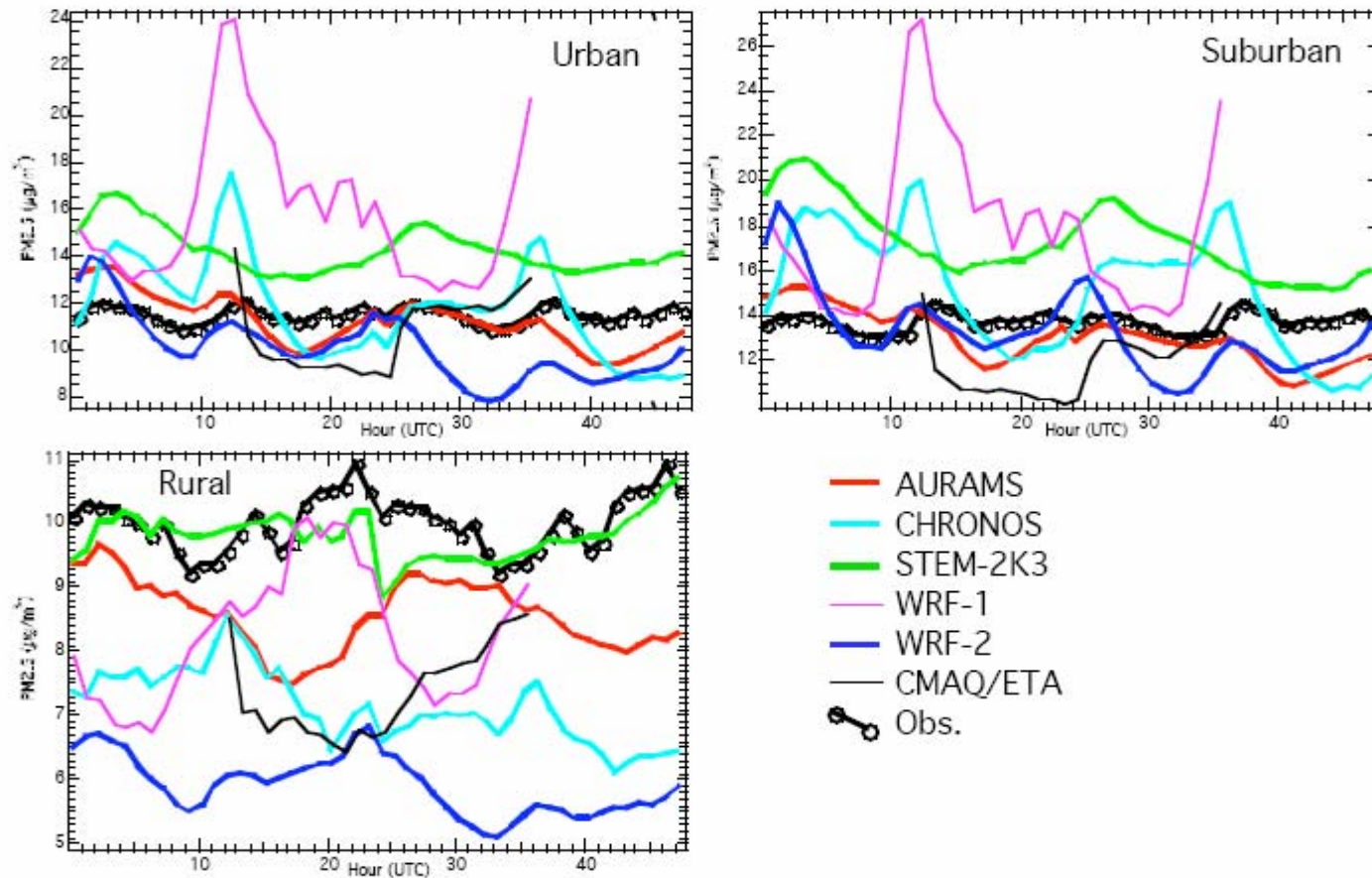


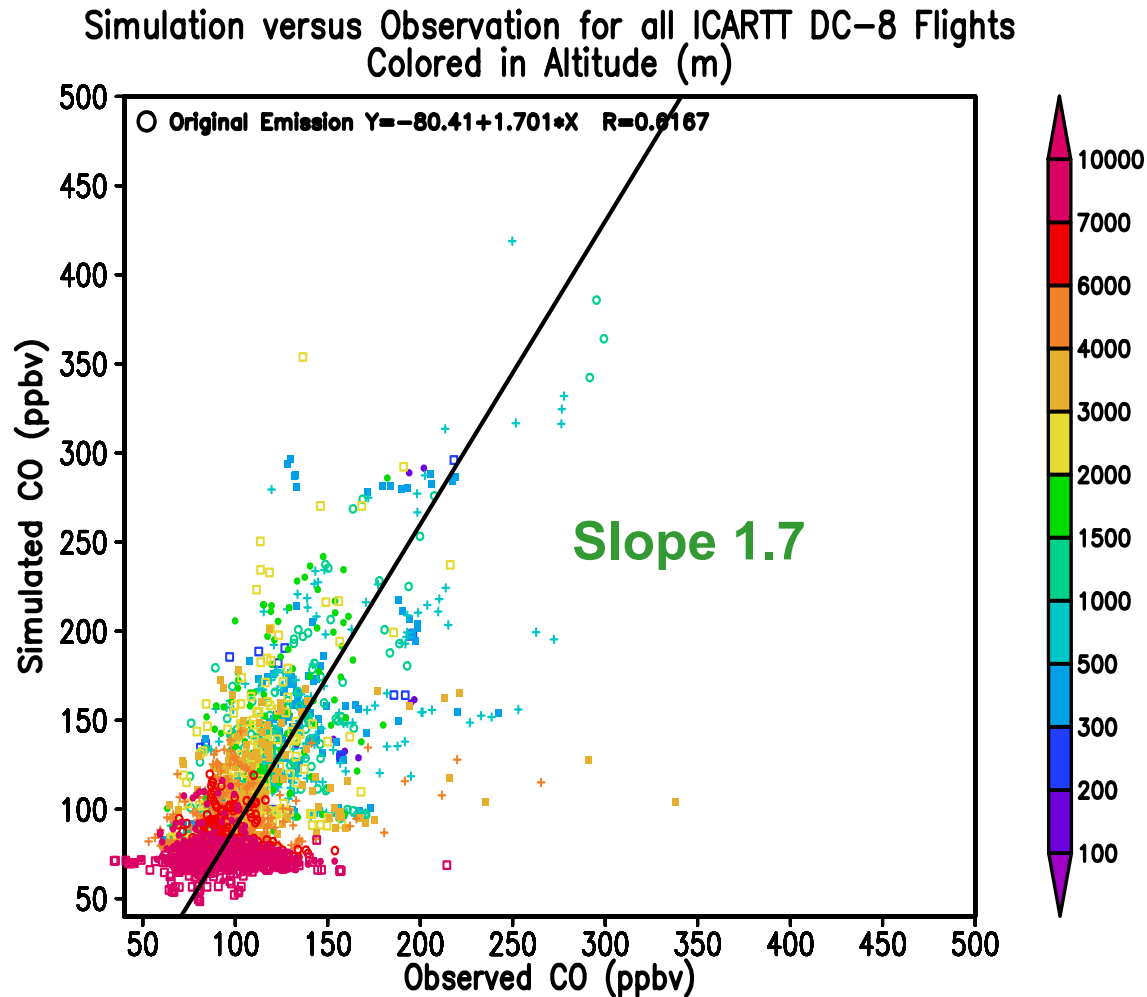
Figure 5. Sorted r-correlation coefficients for the 8 model cases, and persistence

But take little comfort..... We have a long way to go !!

PM_{2.5} Average Diurnal Profiles, summer 2004, in NE U.S.



Emission Issues

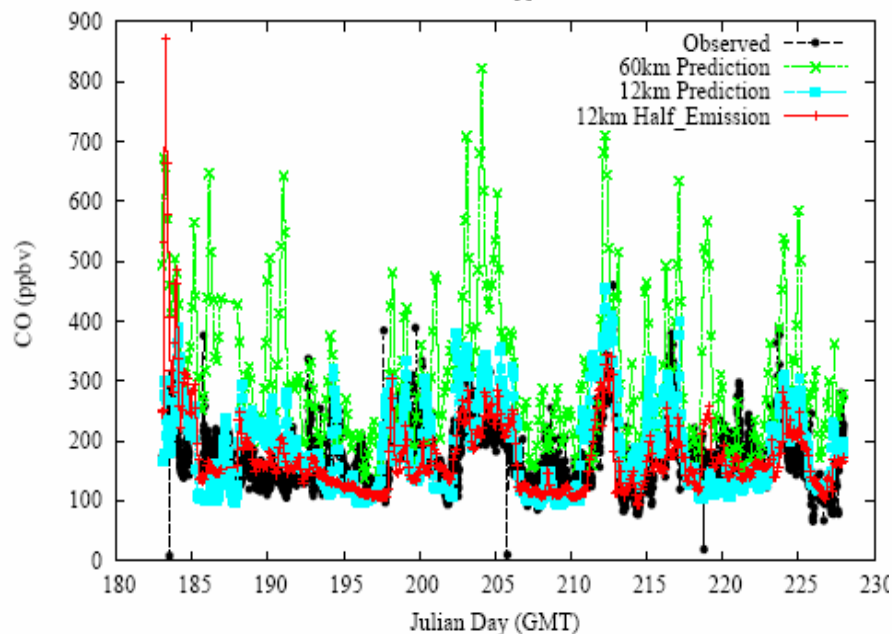


Sensitivity Runs Using Reduced Emissions -- Correlations between STEM simulations and Measurements for All DC-8 flights

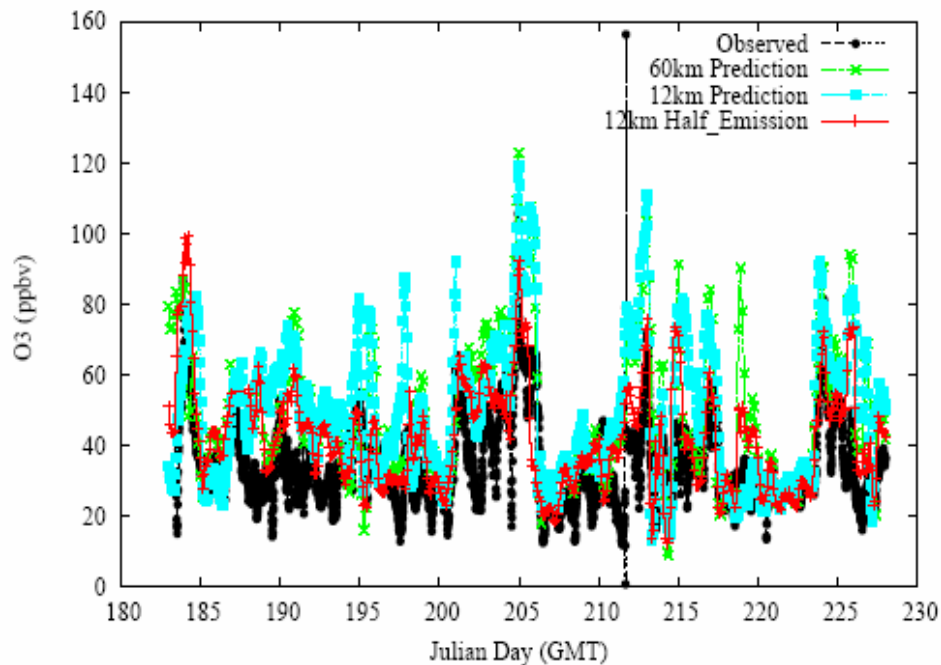
Species	60 km simulation with original NEI-1999v3 emission		60 km simulation with half CO, NO _x and SO ₂ emissions	
	Slope	R	Slope	R
CO	1.70	0.62	0.83	0.66
NO _y	4.11	0.48	1.50	0.48
PILS SO ₄ ²⁻	2.52	0.75	0.78	0.75
SAGA SO ₄ ²⁻	3.06	0.74	1.13	0.74
PILS NH ₄ ⁺	0.35	0.35	0.33	0.48
SAGA NH ₄ ⁺	1.60	0.64	1.08	0.66
O ₃	1.13	0.46	0.97	0.55
Ethyne	0.21	0.50	0.26	0.51
URI HCHO	0.82	0.84	0.89	0.84
H ₂ O ₂	0.56	0.70	0.47	0.67

Clear Improvement in Surface Predictions

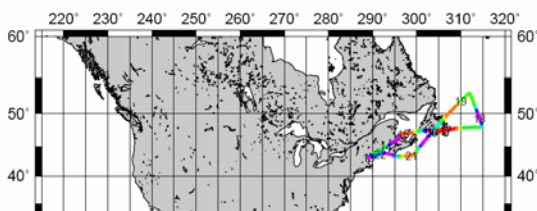
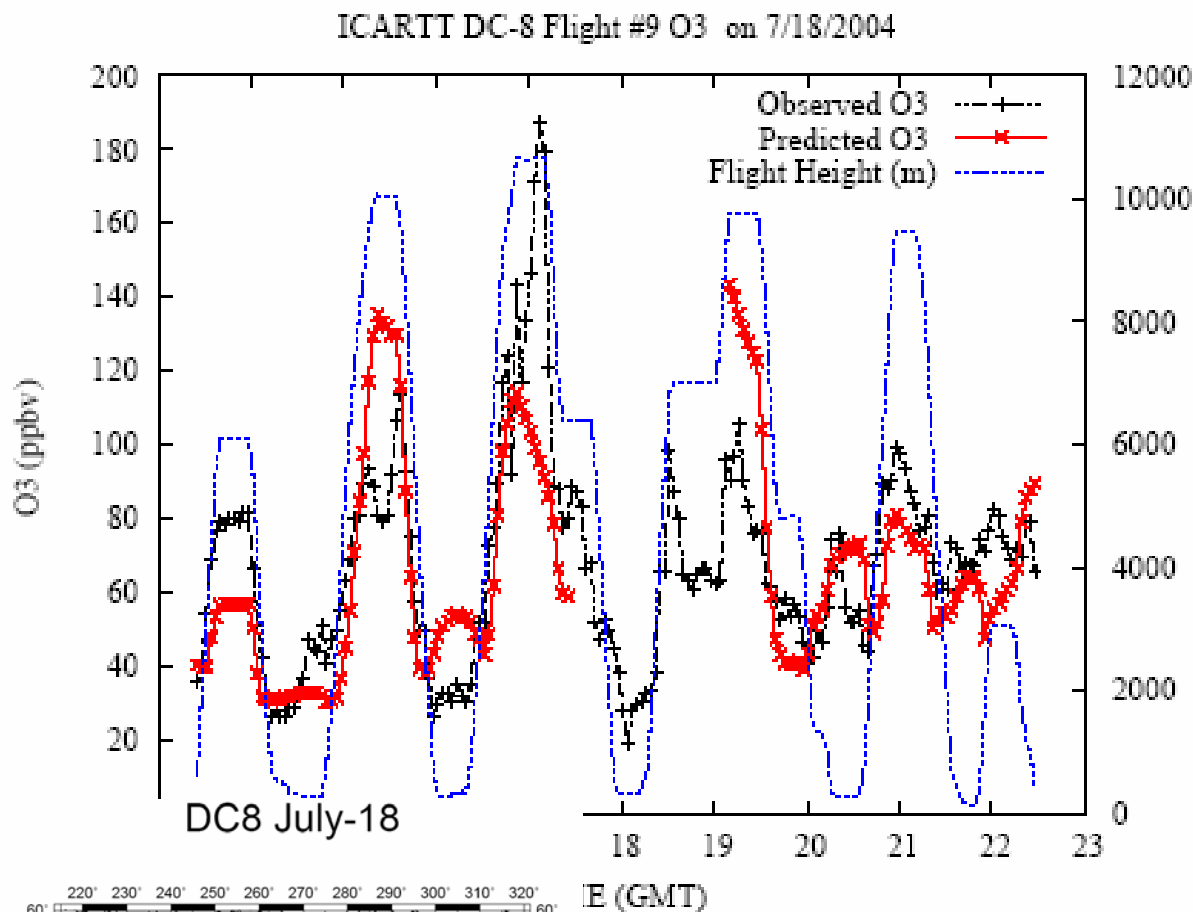
Predicted and Observed CO (ppbv) over Isle of Shoals



Predicted and Observed O3 (ppbv) over Castle Springs



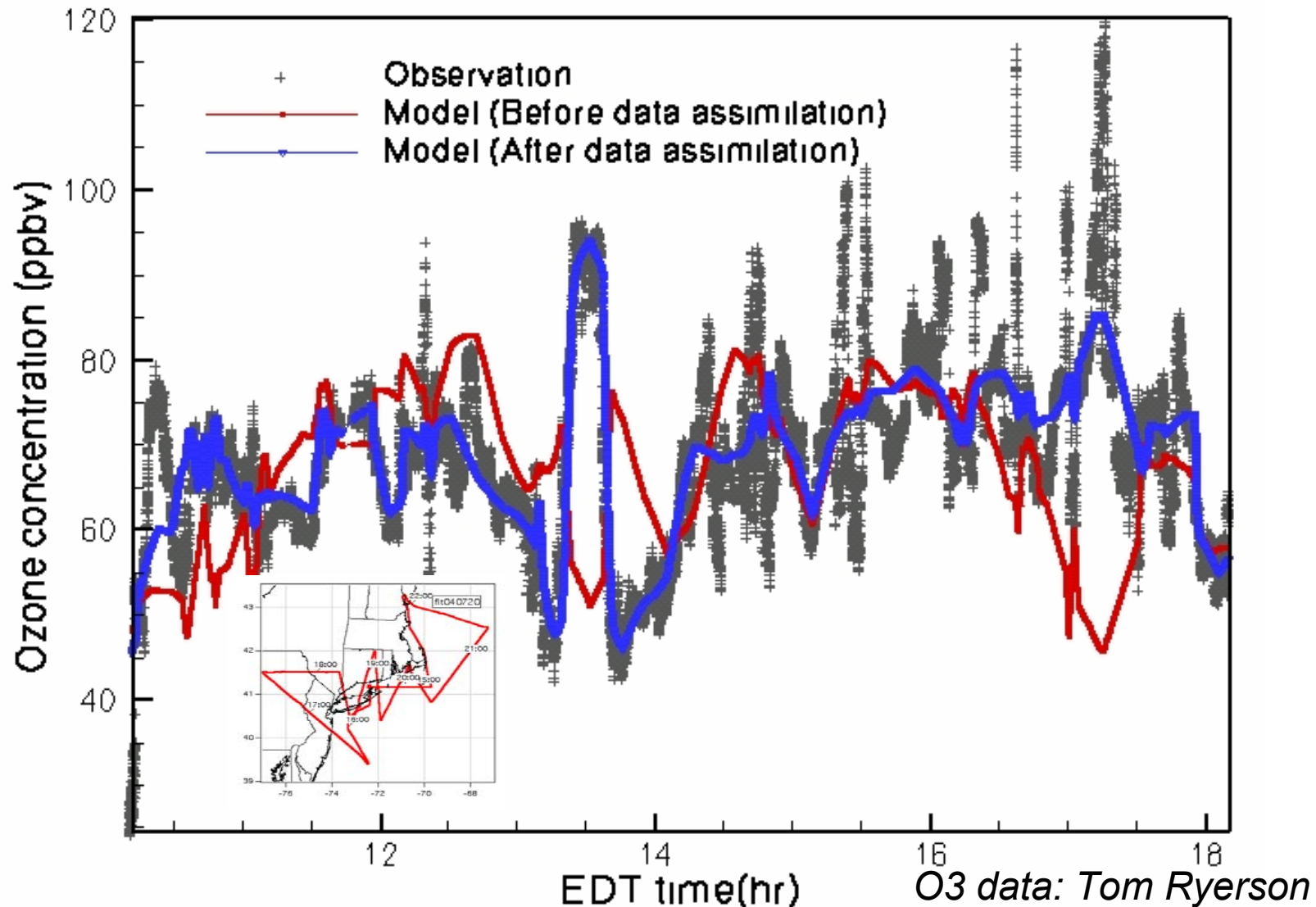
Integration of Measurements & Models



Data: Larc

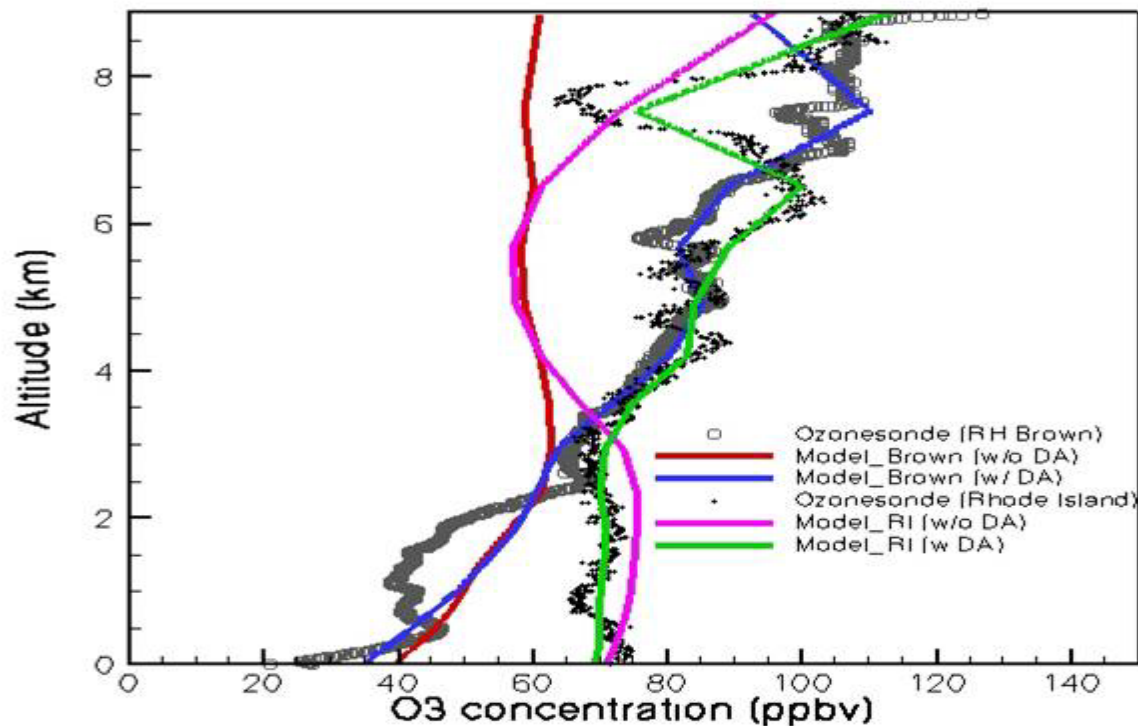
- **Cost functional** measures the model-observation gap.
- **Goal:** produce an **optimal state** of the atmosphere using:
 - Model information consistent with physics/chemistry represented
 - Measurement information consistent with reality
 - *within errors*

Reanalysis of Ozone using Surface as Well as Ozone Profile and Aircraft Data



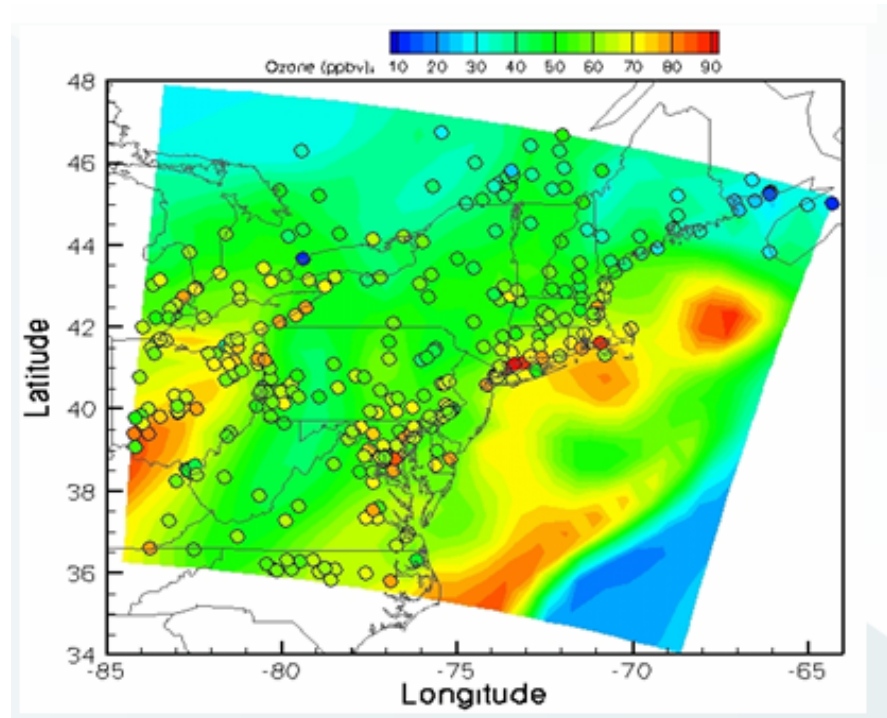
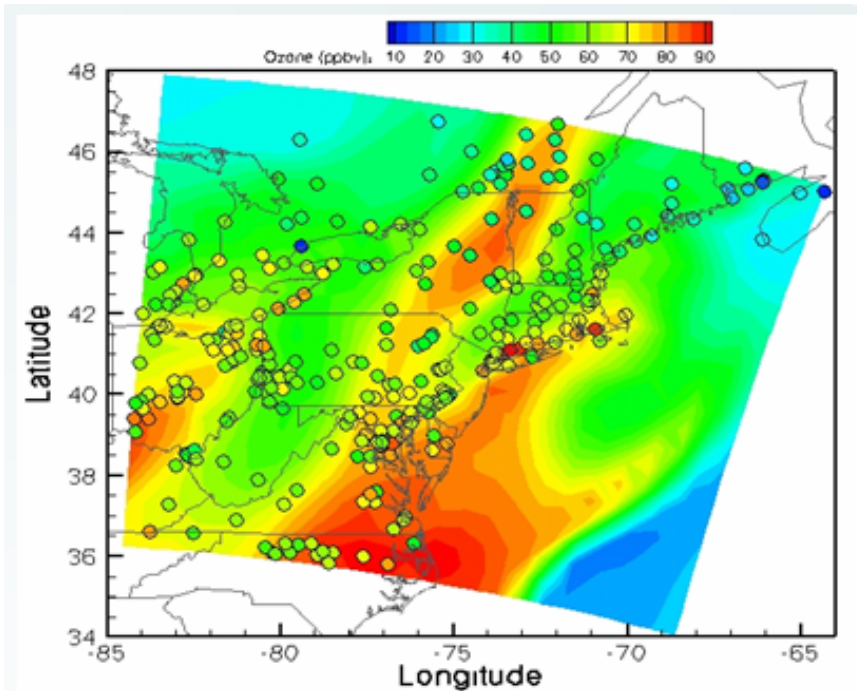
Getting the Vertical Distributions Right is Critical

*Current models have a difficult time...so data
assimilation is important*



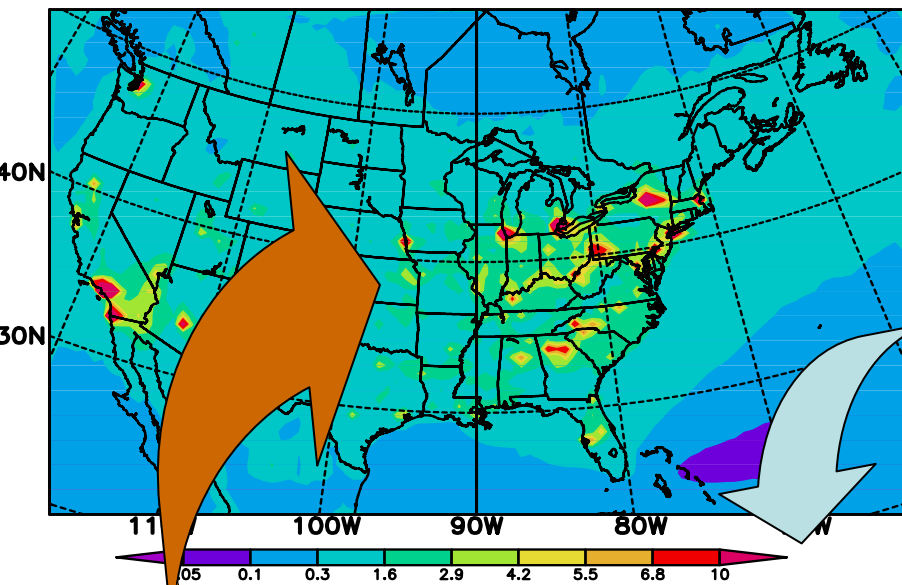
IONS O3 data: Anne Thompson & John Merrill

Ozone Forecasts (*left*) and Reanalysis (*Right*)

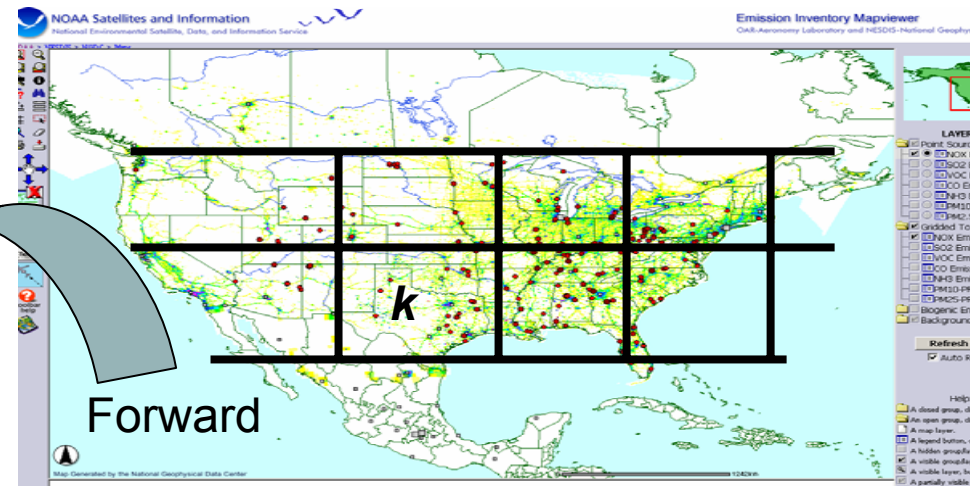


*Circles represent observations
(locations and values)*

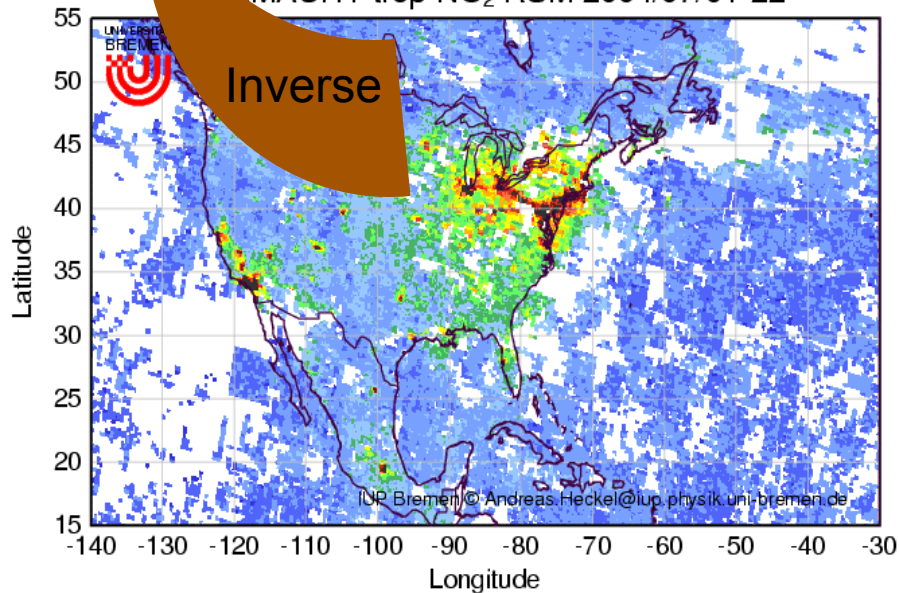
Monthly Averaged Forecasted NO₂ (10^{15} molecules/cm²)



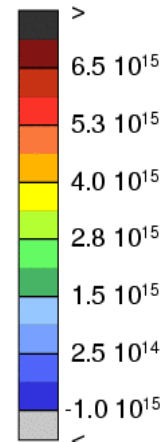
4dVar can be used to recover emissions



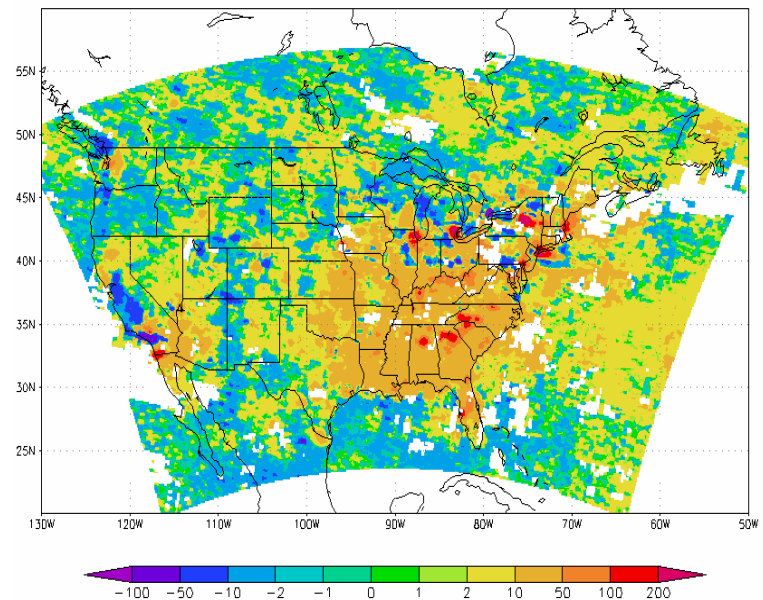
AMACHY trop NO₂ RSM 2004/07/01-22



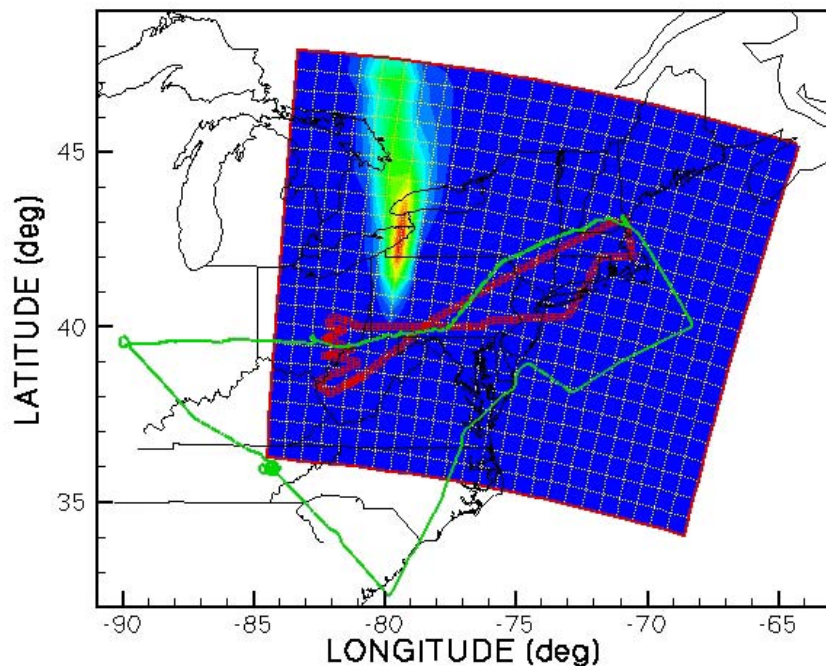
VC NO₂
[molec cm⁻²]



July Averaged NO₂ difference (Model-Obs) (10^{14} Molecules/cm²)

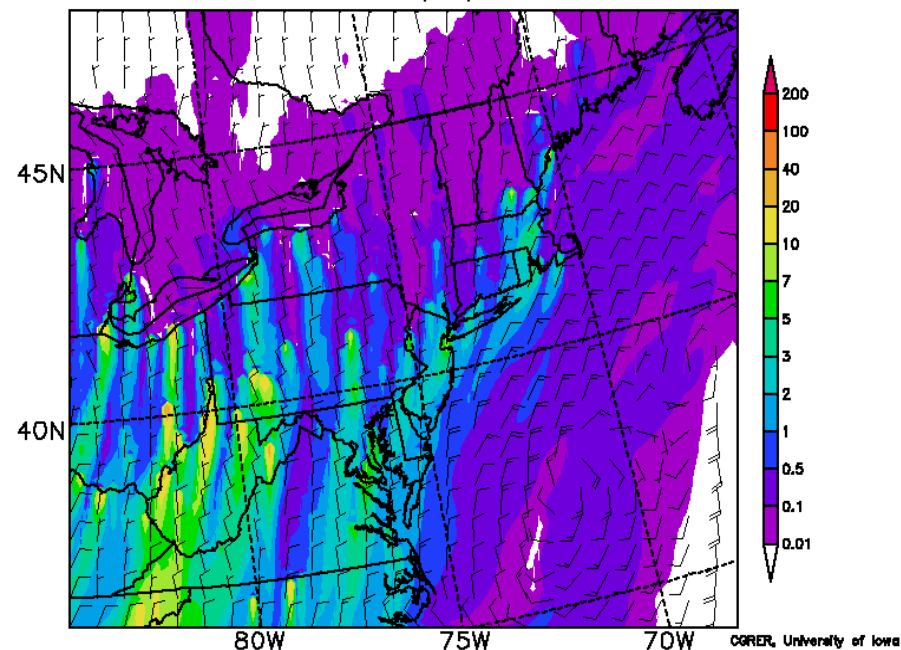


Influence Function



Adjoint Tools Can Also
Help in the
Characterization of
Emissions

Simulated SO_2 (ppbv) in the 400m layer
at 21GMT, 08/06/2004

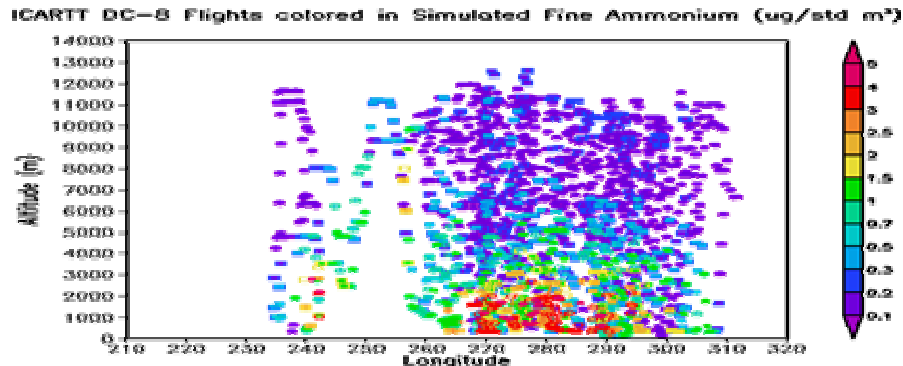
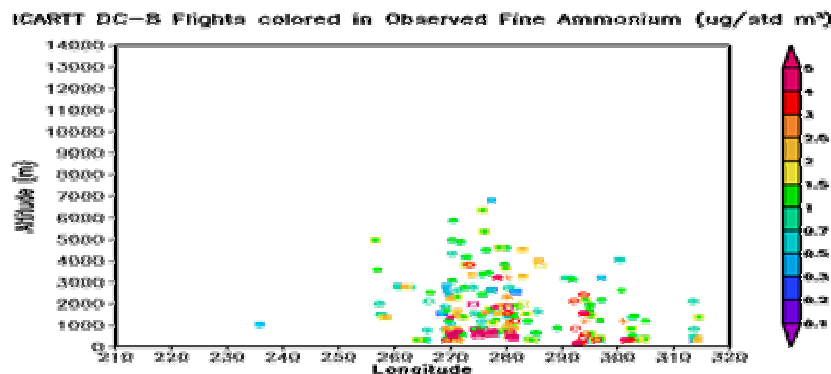
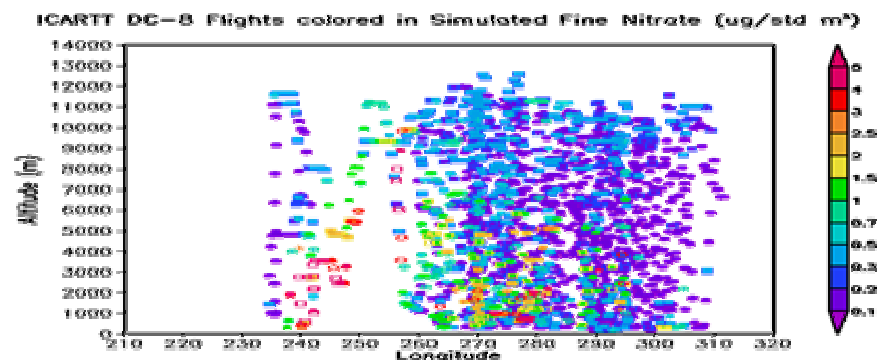
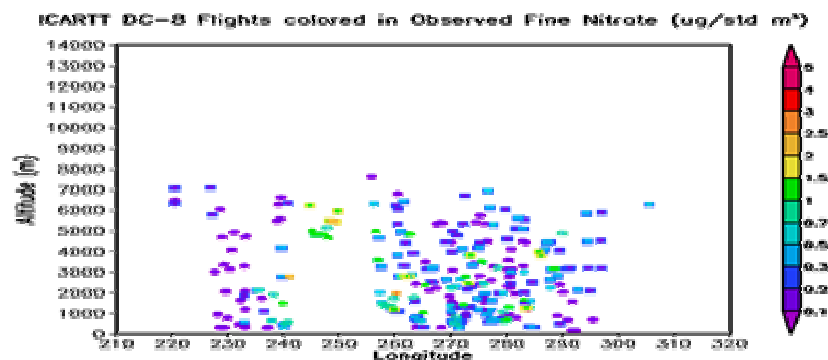
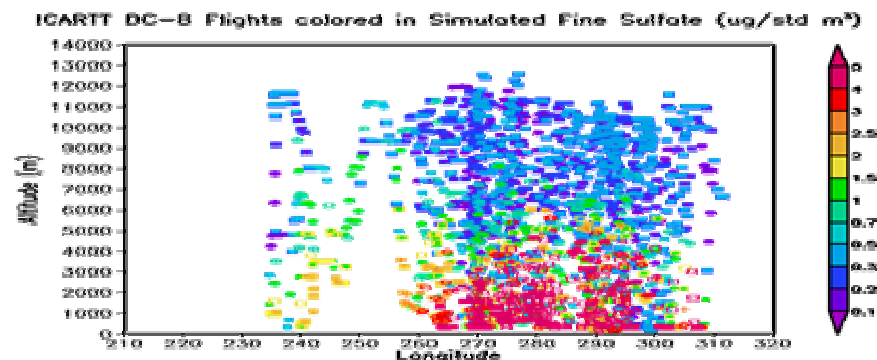
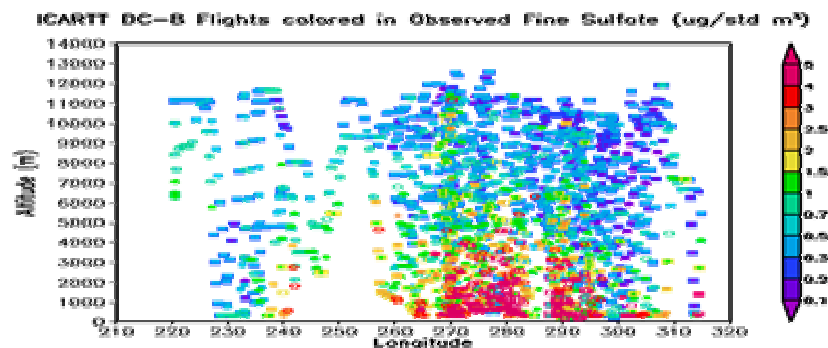


**Preliminary Results: CO
emission scaling factor
~ 0.7.**

Regional Distributions of Aerosols

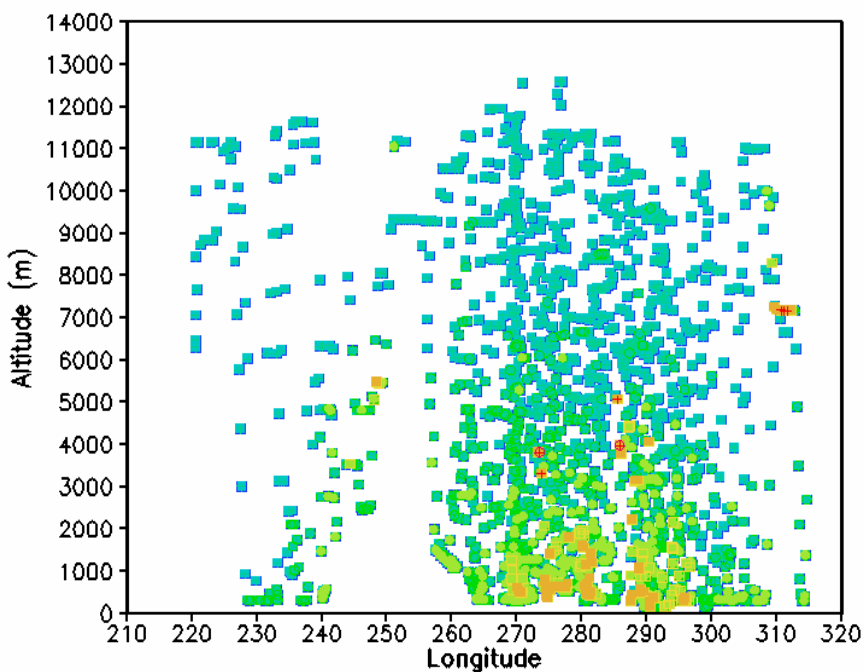
Observed (PILS)

Predicted

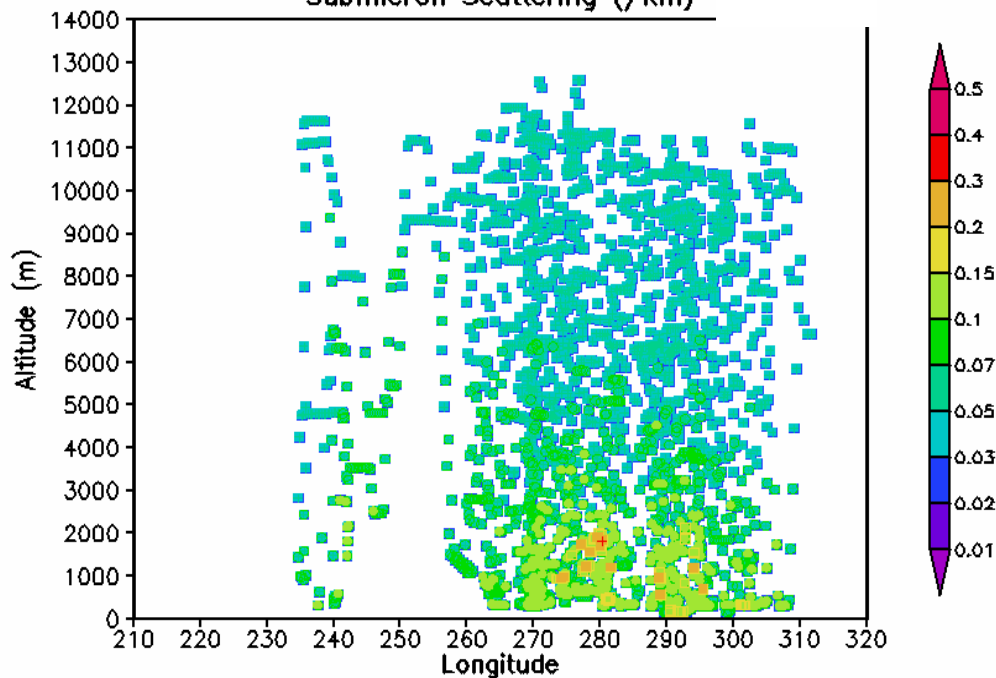


Observed and Predicted Submicron Scattering

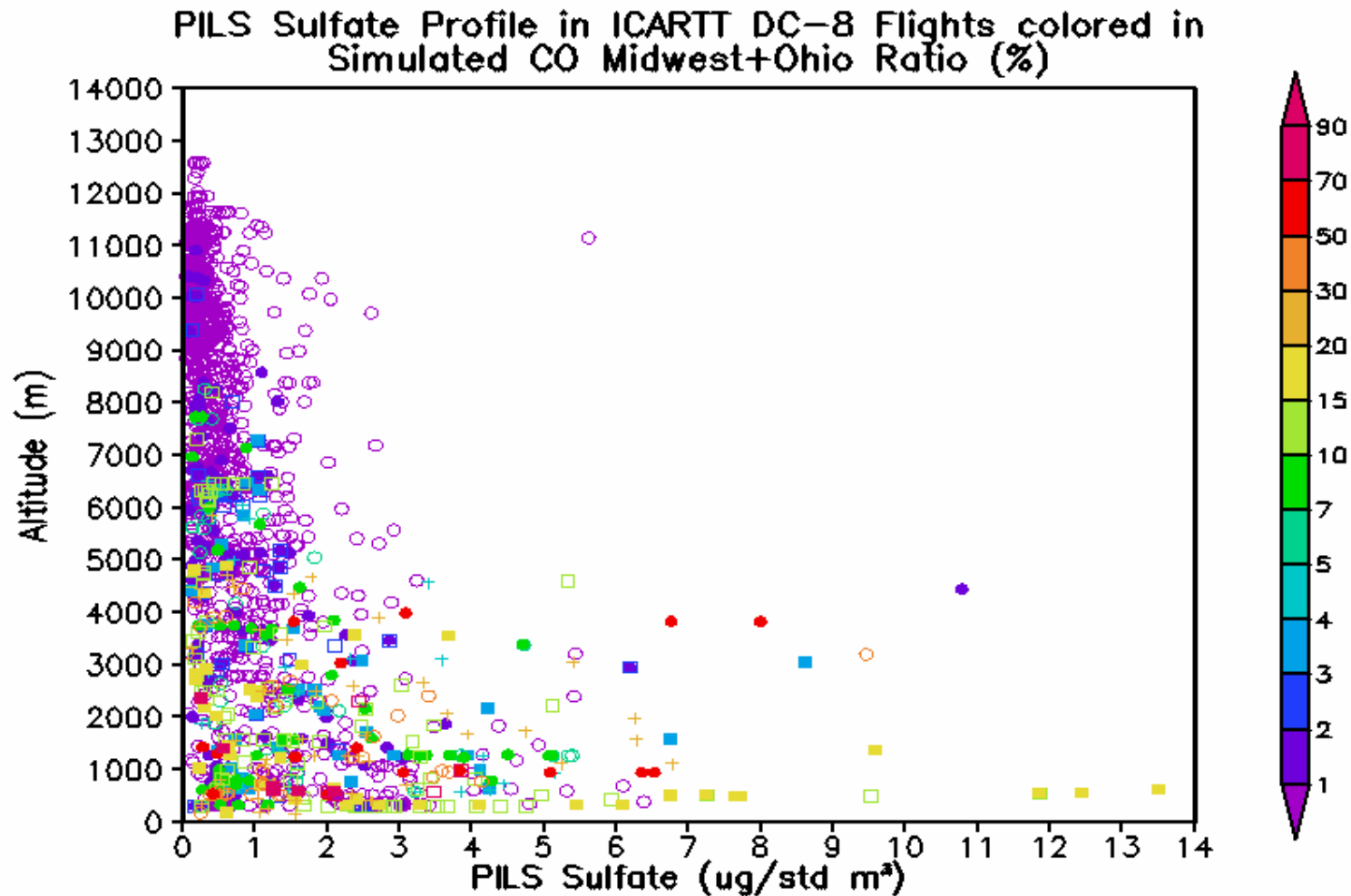
ICARTT DC-8 Flights colored in Observed Submicron Scattering



ICARTT DC-8 Flights colored in Simulated Submicron Scattering (/km)



STEM Source Region Tracers Can Be Used to Sort Data & Complement Trajectories



Future Plans

- Improve Base Emissions -- Update base year inventory (Streets and Vukovich), Biomass burning (others)
- Emission inversions
- Re-analysis using aircraft, surface, satellites, sondes (Ozone, CO, NO_y, HCHO)
- Analysis of aerosols and optical properties, by better linking observations and models
- Better understand and constrain physical removal processes (dry and wet)

We will submit our model products along the flight tracks